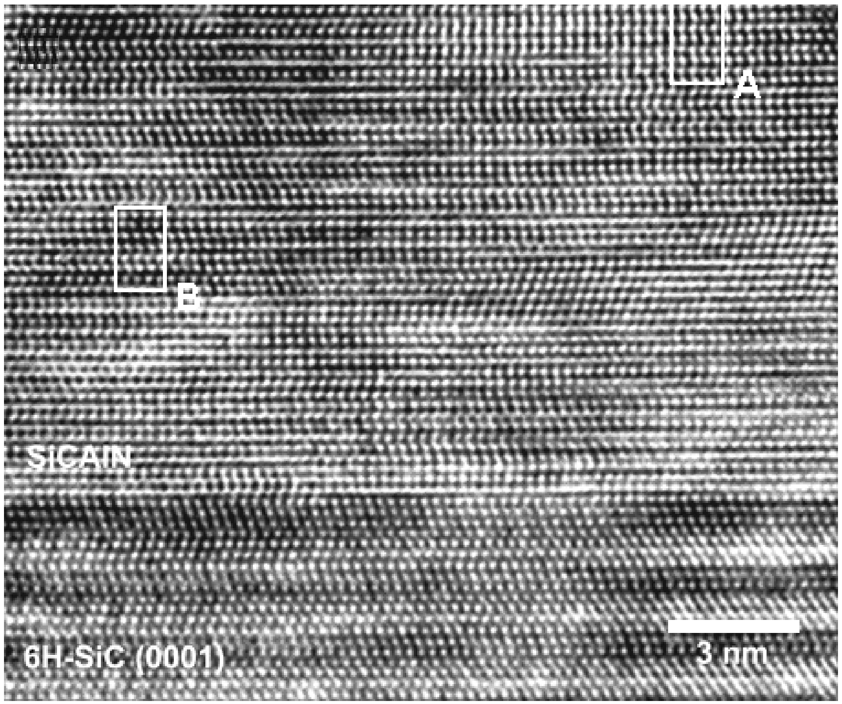
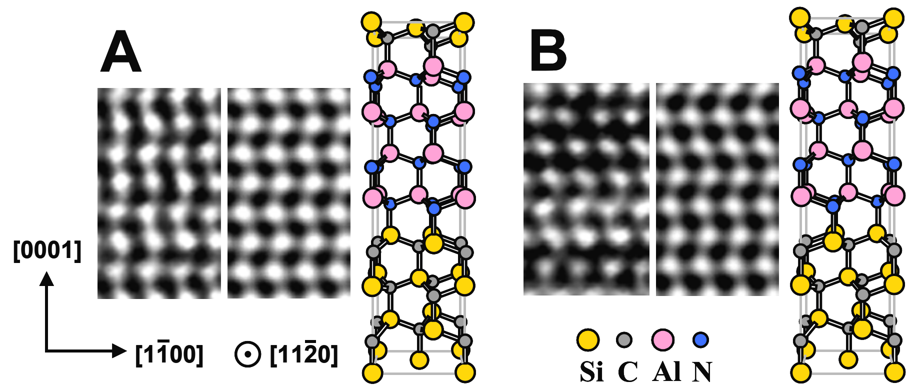
New Pseudo-binary Wide Band Gap Semiconductor SiCAlN



High-resolution XTEM image of SiCAlN grown on 6H-SiC(0001) substrate. Two outlined regions A and B are selected for computer-simulated image matching.



Comparison of XTEM image (left) with simulated image (right) based on unit cells of 2H-SiC and 2H-AlN for region A, and 4H-SiC and 2H-AlN for region B.

DMR-9986271, Tailoring Surface Morphology in Group III Nitride Heteroepitaxy,

P.I. : I.S.T. Tsong

Two compounds, SiC and AlN, normally insoluble in each other below ~2000^{o}C, are synthesized as a single-phase solid-solution thin film by molecular beam epitaxy (MBE) at 750^{o}C. The growth of epitaxial SiCAlN films with hexagonal structure takes place on 6H-SiC(0001) substrates using a flux of H_3SiCN gaseous unimolecular precursor and an Al flux from an effusion cell. Two structural models for the hexagonal SiCAlN are constructed based on first-principles total-energy density functional theory calculations, each showing agreement with the experimental microstructures observed in cross-sectional transmission electron microscopy (XTEM) images. Regions outlined as A and B in the high-resolution XTEM image are compared with computer-simulated images based on the SiCAlN structure comprising unit cells of 2H-SiC and 2H-AlN (A), and unit cells of 4H-SiC and 2H-AlN (B). Good image matching is observed between the experimental image (left) and the simulated image (right) for both regions A and B. The theoretical predicted fundamental band gap for the SiCAlN film is 3.2 eV, in good agreement with room-temperature photoluminescence measurements. Theoretical calculations of the variation of band gap with composition suggests that band-gap engineering between 3.2 and 4.5 eV is attainable simply by increasing the AlN content in the film from 50% to 75%. The results are published in Phys. Rev. Lett. **88**, 206102 (2002). The approach of combining a custom-designed unimolecular precursor and metal atoms presents a direct way to grow new metastable pseudo-binary semiconductors in the XCZN family, where X is a Group IV metal and Z is a Group III metal. Hypothetical semiconductors with adjustable band gaps, such as GeCGaN, are within reach.

NSF Outcome Goal for People

DMR-9986271
PI: I.S.T. Tsong

Interdisciplinary and International Collaborations

The new results on the pseudo-binary wide band gap semiconductor SiCAlN were obtained from a collaboration with Dr. John Kouvetakis, Professor of Chemistry at Arizona State University, who is also supported by NSF-DMR (Solid State Chemistry). One of graduate students on the project, Radek Roucka, was a visiting scholar from the Czech Republic supported jointly by DMR and the Division of International Programs (DMR-958513) and he had elected to stay in Arizona State University to complete a Ph.D. program in Science and Engineering of Materials. Mr. Roucka is the lead author in our paper on SiCAlN published in Phys. Rev. Lett. **88**, 206102 (2002).